

TOPIC 04 – BONDING

4.2 – COVALENT BONDING

IB Chemistry
T04D02



4.2

Covalent Bonding I

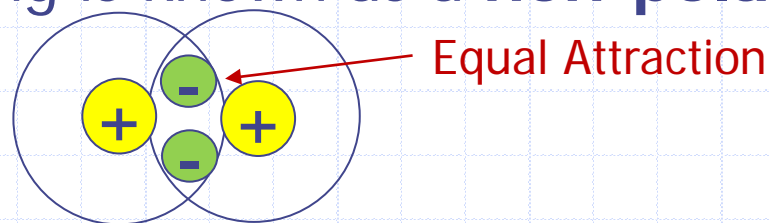
- 4.2.1 Describe the covalent bond as the electrostatic attraction between a pair of electrons and positively charged nuclei. (2)
- 4.2.2 Describe how the covalent bond is formed as a result of electron sharing. (2)
- 4.2.3 Deduce the Lewis (electron dot) structures of molecules and ions for up to four electron pairs on each atom. (3)
- 4.2.4 State and explain the relationship between the number of bonds, bond length and bond strength. (3)
- 4.2.5 Predict whether a compound of two elements would be covalent from the position of the elements in the periodic table or from their electronegativity values. (3)
- 4.2.6 Predict the relative polarity of bonds from electronegativity values. (3)
- 4.2.7 Predict the shape and bond angles for species with four, three and two negative charge centers on the central atom using the valence shell electron pair repulsion theory (VSEPR). (3)
- 4.2.8 Predict whether or not a molecule is polar from its molecular shape and bond polarities. (3)
- 4.2.9 Describe and compare the structure and bonding in the three allotropes of carbon (diamond, graphite and C₆₀ fullerene). (3)
- 4.2.10 Describe the structure of and bonding in silicon and silicon dioxide. (2)



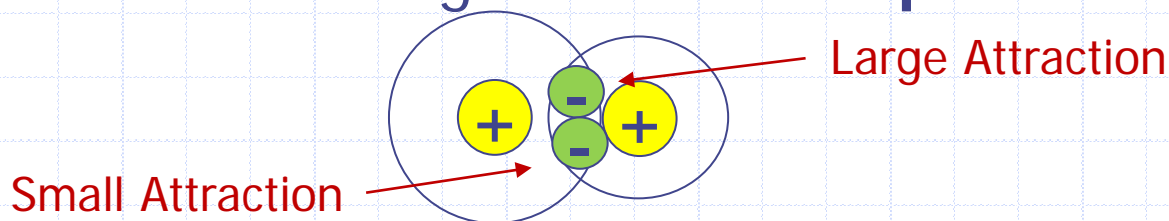
4.2 Definition of a Covalent Bond

4.2.1 Describe the covalent bond as the electrostatic attraction between a pair of electrons and positively charged nuclei. (2)

- A **covalent bond** is known as the electrostatic attraction between a pair of electrons and positively charged nuclei
- The simplest example is H_2 (a non-polar covalent compound)
 - Held by the attraction of each nucleus to the shared pair
 - The equal sharing is known as a **non-polar covalent bond**



- When atoms have different sizes, and hence electronegativity, the smaller atom will attract electrons more strongly (less electron shielding)
 - The uneven sharing is known as a **polar covalent bond**

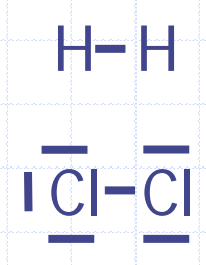
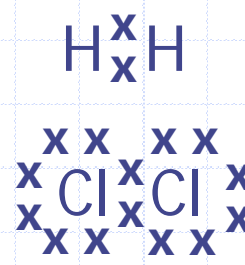
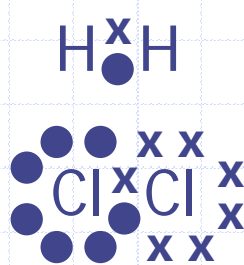
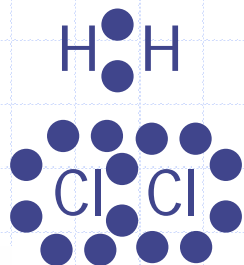


4.2

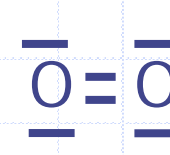
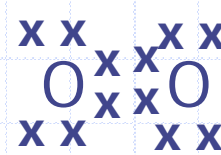
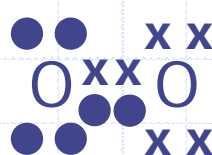
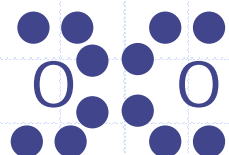
Covalent Bond Formation

4.2.2 Describe how the covalent bond is formed as a result of electron sharing.

- In a single bond, each atom contributes one electron (unless dative) to the shared pair.
- Each atom then achieves noble gas configuration
- When two or more atoms are joined by covalent bonds the species is then known as a **molecule** or a **molecular compound**.
- Covalent bonds are generally formed between non-metals
- Diatomic Molecules (Br_2 , I_2 , N_2 , Cl_2 , H_2 , O_2 , F_2) known as "BrinClhof," are examples of covalently bound molecules



SINGLE
 Cl_2 H_2

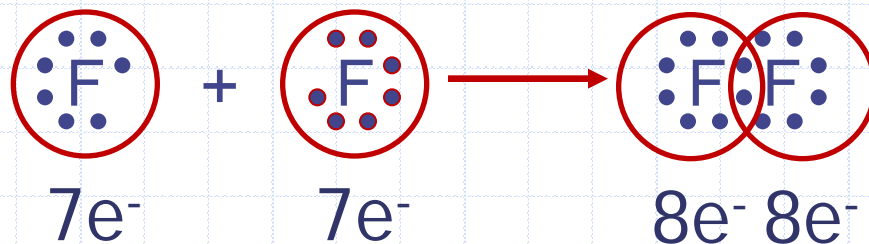


DOUBLE
 O_2

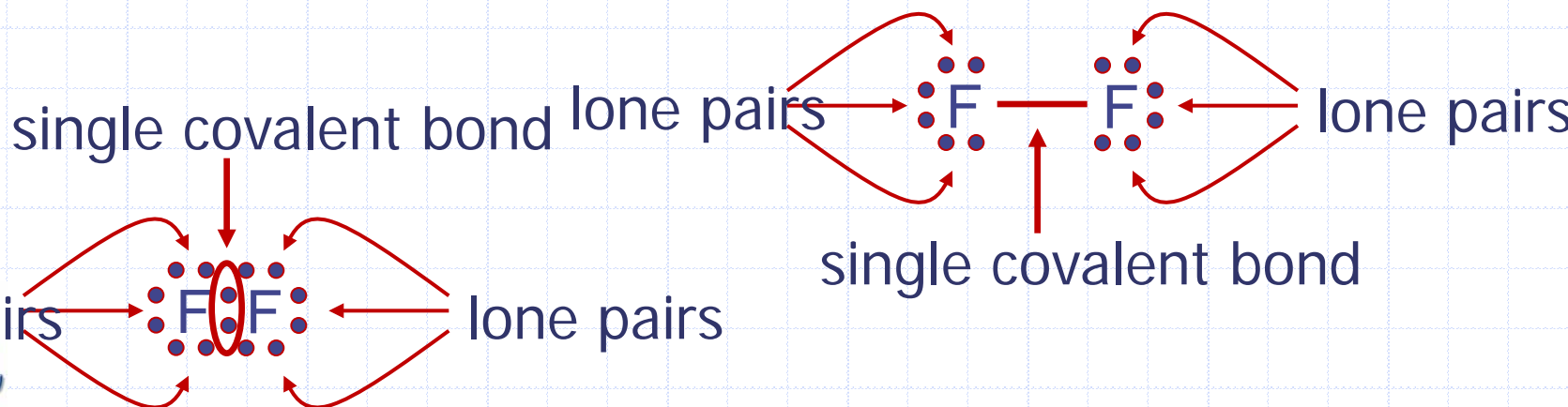


More examples of Covalent Bond formation: Mr. Martin Brakke

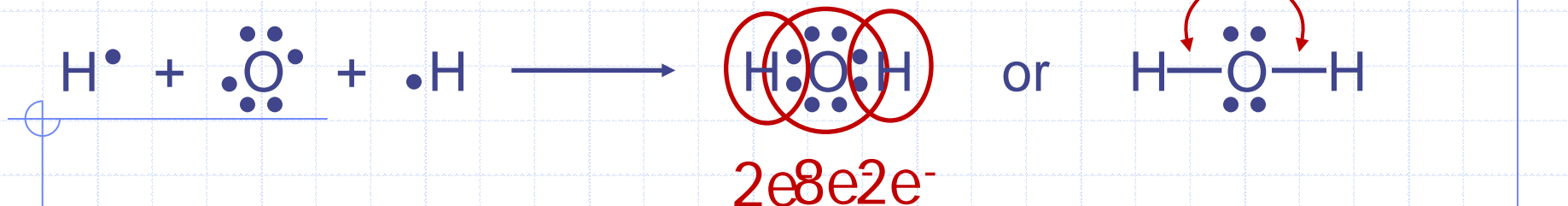
- Most** elements will complete the "**octet rule**," except H and He completing the "**duet rule**," and other exceptions (such as S and P which have an expanded octet)



Lewis structure of F_2



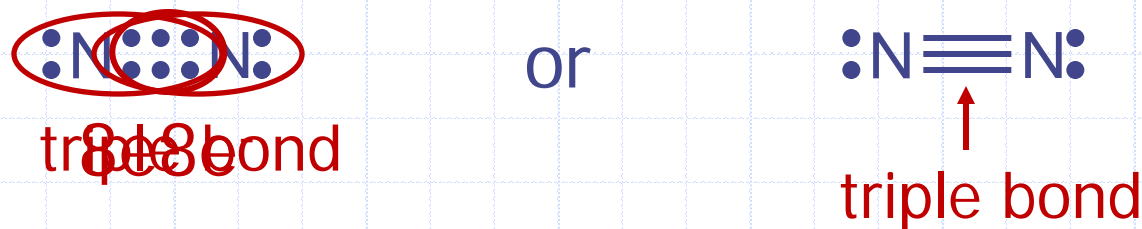
Lewis structure of water



Double bond – two atoms share two pairs of electrons



Triple bond – two atoms share three pairs of electrons



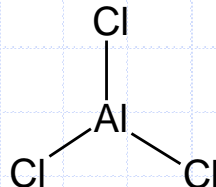
Exceptions to the Octet Rule

- Duet Rule: Hydrogen and Helium (and any cation with an He configuration) only need 2 electrons to complete the stability requirements for the first shell
- Common exceptions include:

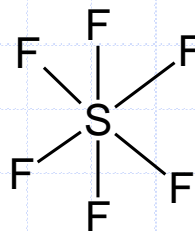
- Beryllium (BeCl_2)



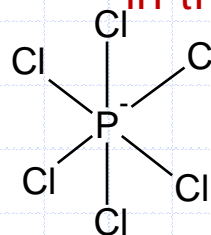
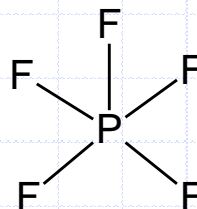
- Aluminum (AlCl_3)



- Sulfur (SF_6)



- Phosphorous (PF_5 or PCl_6^-)



Incomplete Octet:
Elements in Period 2 cannot surpass the octet rule as their outer shell cannot hold more than 8. These are known as **electron deficient**.

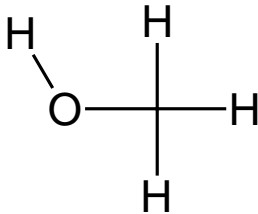
Expanded Octet: Have more than 8 electrons as elements in Period 3 can have up to 18 electrons in their outer shell



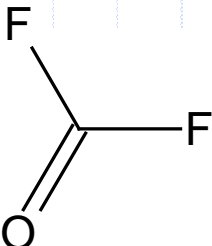
Valency of Elements

- The **valency** is a measure of the number of chemical bonds formed by the atoms of a given element.
- This may also be known as **combining power**
 - Applied to the formation of molecules by non-metals
 - Is based on the **formal charge** (which we may cover later) where elements are most stable with a formal charge of zero

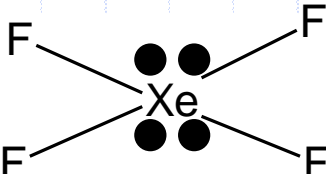
H 1																	He	
Li 1	Be 2											B 3	C 4	N 3	O 2	F 1	Ne	
Na 1	Mg 2											Al 3	Si 4	P 3/5	S 2/4/6	Cl 1	Ar	
K 1	Ca 2	Sc 3	Ti 4	V 3/4/5	Cr 3/6	Mn 2/4/7	Fe 2/3	Co 2	Ni 2	Cu 1/2	Zn 2				Br 1	Kr		
Rb 1	Sr 2											Ag 1		Sn 2/4			I 1	Xe 6
Cs 1	Ba 2													Pb 2/4				



O



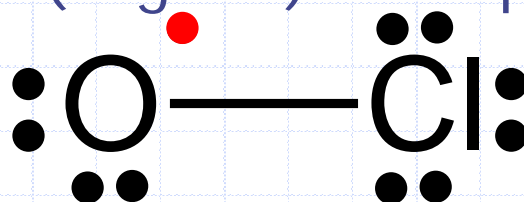
O=C=O



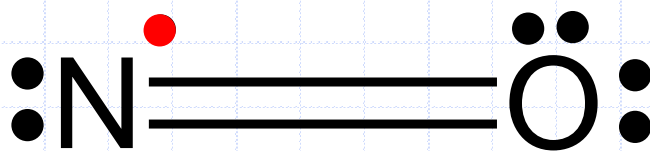
F6Xe

Free Radical Molecules

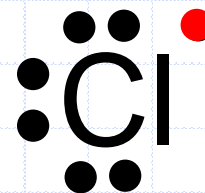
- Stable molecules contain even numbers of electrons
- There are some molecules that (although reactive) can exist with an odd number of electrons
- These are called **free radicals** as they have an unpaired electron
 - This will not be significant in this unit but will come back around in Topic 10 (Organic) and Option E (Environmental)



Oxy-chlorine radical: formed as an intermediate during the destruction of Ozone



Nitrogen monoxide

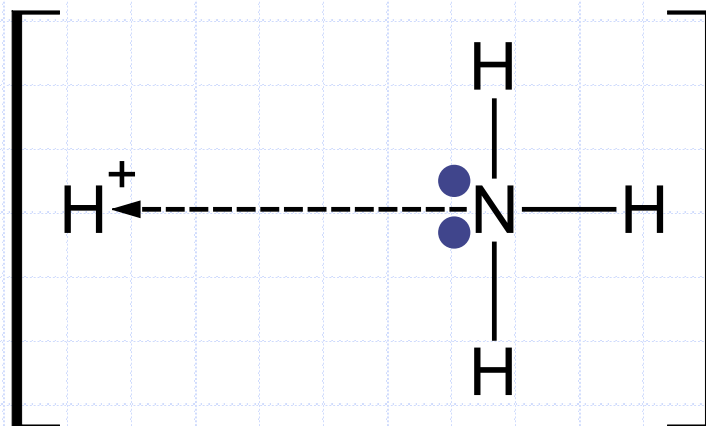


Chlorine radical: formed as Cl_2 comes in the presence of uv light which initiates the substitution of Cl into an alkane



Coordinate Covalent Bonds

- When both electrons that are shared (in a single bond) come from the same atom, the bond is known as a **coordinate bond** or a **dative bond**.
 - Shown as an arrow (\rightarrow) instead of a bond (-) where the electrons came from the source of the arrow
 - The **coordination number** is the number of bonds (to **ligands**) formed around the central atom
 - In Topic 08 (Acids and Bases) known as **Lewis acids and bases**



4.2

Lewis Dot Structures

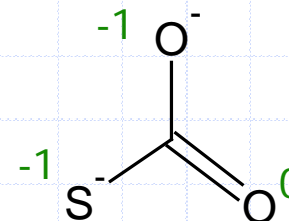
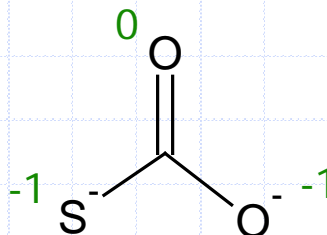
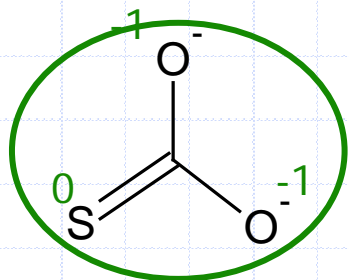
4.2.3 Deduce the Lewis (electron dot) structures of molecules and ions for up to four electron pairs on each atom. (3)

- In general for drawing Lewis structures
 - Determine total # valence electrons available
 - Central atom is the least electronegative (NOT Hydrogen)
 - Draw one bond to each terminal atom
 - Place remaining electrons as lone pairs on terminal atoms
 - Form multiple bonds if there is not enough electrons
- A very simple rule can be used to determine the number of bonds in a molecule: **The NAS rule:**
 - **$N - A = S$**
 - N = Total electrons **needed**, duet or octet (2 or 8)
 - A = Valence electrons **available**
 - S = **Shared** electrons (divide by 2 for bonds)



Formal Charge

- When deciding between various structures, the most stable can be found by determining the formal charge of each element
- The **formal charge** of an atom is the number of valence electrons in the free atom minus the number of electrons assigned to that atom
 - Formal Charge = (# Valence) – [(# Bonds) + (# Lone e⁻)]**
- For Example, in CSO_2^{2-} , the most stable is:



For Sulfur:

- When S = $\text{FC} = 6 - (2 + 4) = 0$
- When S⁻ $\text{FC} = 6 - (1 + 6) = -1$

For Oxygen:

- When O = $\text{FC} = 6 - (2 + 4) = 0$
- When O⁻ $\text{FC} = 6 - (1 + 6) = -1$

O is more electronegative, hence it is more stable with the F.C. of -1



4.2

Bond Length and Strength

4.2.4 State and explain the relationship between the number of bonds, bond length and bond strength. (3)

Length of Bonds:

- The more shared pairs of electrons between nuclei, the closer they will attract each other, therefore:
- Triple < Double < Single

Strength of Bonds:

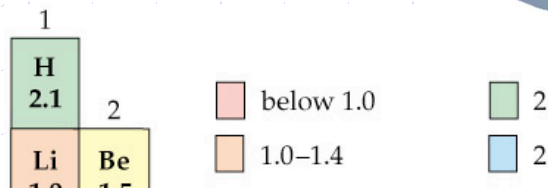
- Stronger attraction to pull bonds closer also explains the trend in bond strength:
 - Single < Double < Triple
- Stronger bonds = shorter bonds

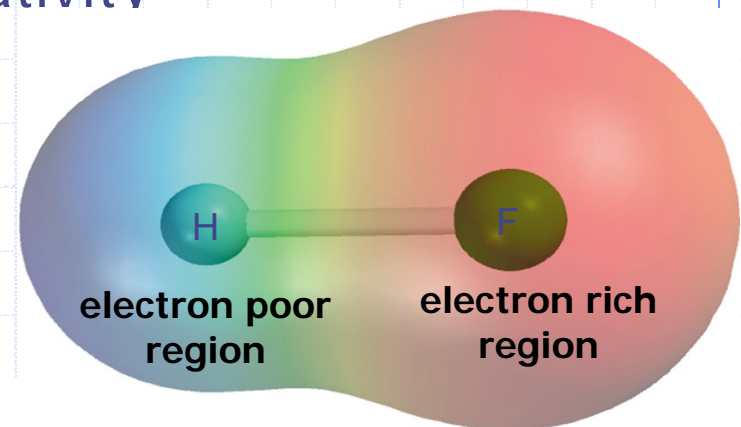
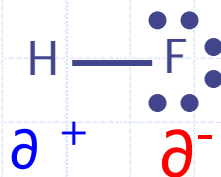
Bond Type	Bond Enthalpy (kJ mol ⁻¹)	Bond Length (nm)
Single (C-C)	348	0.154
Double (C=C)	612	0.134
Triple (C≡C)	837	0.120



Bonding Type Determination

4.2.5 Predict whether a compound of two elements would be covalent from the position of the elements in the periodic table or from their electronegativity values. (3)

- Rough range difference in electronegativity
 - 0 is Non-Polar Covalent
 - Even sharing
 - $0 < \text{Diff} < 1.8$ is Polar Covalent
 - Uneven sharing
 - $\text{Diff} > 1.8$ is Ionic
 - transfer of electrons
- 

[illegible]

4.2

Calculating the Polarity of Bonds

4.2.6 Predict the relative polarity of bonds from electronegativity values. (3)

- If two elements have the same electronegativity values, such as in N_2 , O_2 or F_2 they will be completely **NON-POLAR**
- As soon as one element has a slightly smaller radius due to an increase in the nuclear charge (compared to electron shielding), that element then has a stronger attraction for electrons (electronegativity) and the molecule begins to become **POLAR**
- As one element becomes increasingly stronger, the **IONIC CHARACTER** increases as the bonds become more polar.
- Eventually, if the electronegativity difference increases enough, there is a transfer of the shared electron and the bond becomes **IONIC**

As you can see, there are no discreet points. Even something slightly polar has ionic character

NON-POLAR

POLAR

IONIC



IONIC CHARACTER

4.2 VSEPR and Molecular Geometry

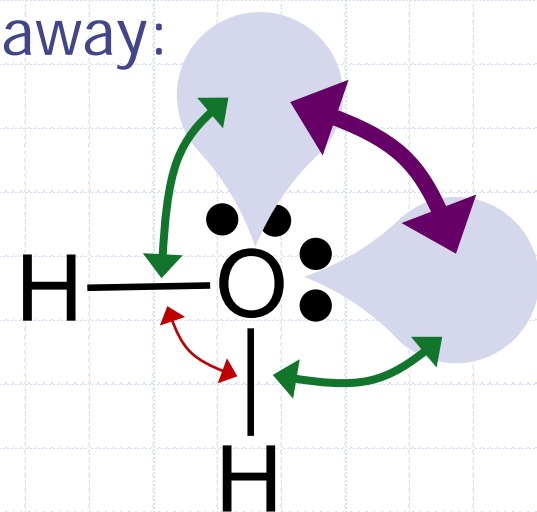
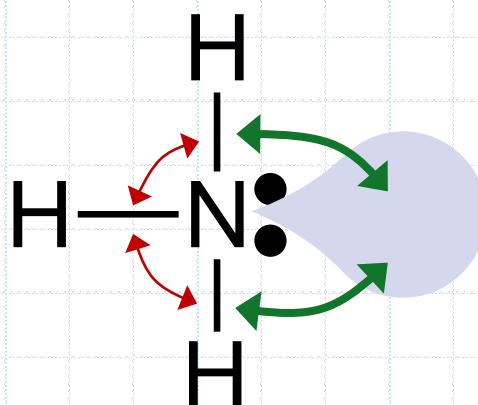
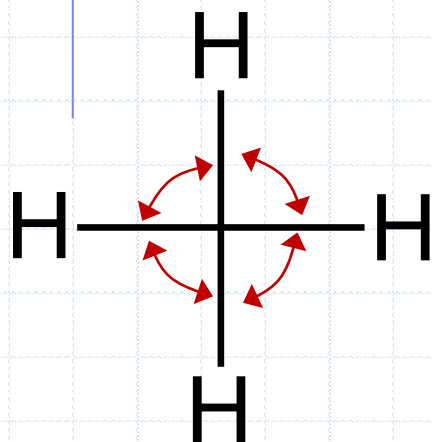
4.2.7 Predict the shape and bond angles for species with four, three and two negative charge centers on the central atom using the valence shell electron pair repulsion theory (VSEPR). (3)

- The shapes of molecules and ions can be predicted by the **Valence Shell Electron Pair Repulsion Theory (VSEPR)**. It states that:
 - The electron pairs around the central atom repel each other
 - Bonding pairs and lone pairs of electrons arrange themselves to be as far apart as possible as to limit electron repulsions
 - Bonding pairs (shared) and Lone pairs (unshared) are termed negative charge centers
 - Shapes are determined by the electron pairs rather than by the atoms



Electron Repulsions

- When electrons are in bonds, the atoms there attached to bring some stability as the nucleus has protons
- When electrons are as lone pairs, there are greater repulsions as the raw charge pushes bonds away:

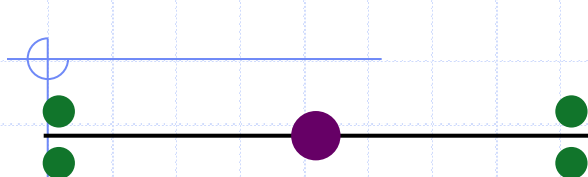


BOND PAIR - BOND PAIR < BOND PAIR - LONE PAIR < LONE PAIR - LONE PAIR

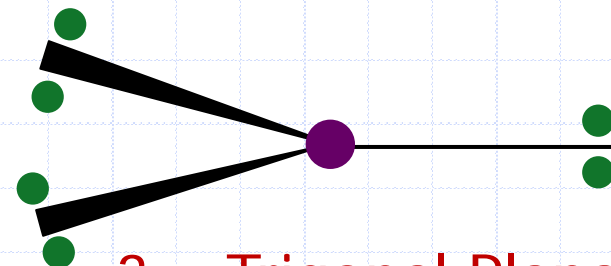


This is all 2D, when we go 3D we must take this into account!

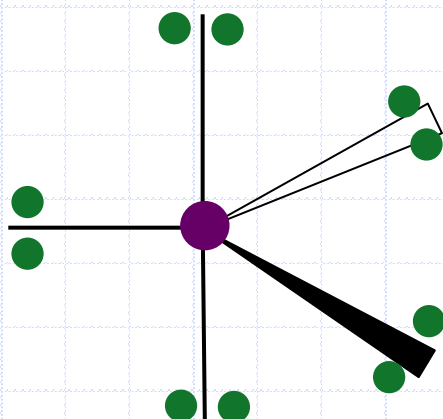
Negative Charge Center Orientation



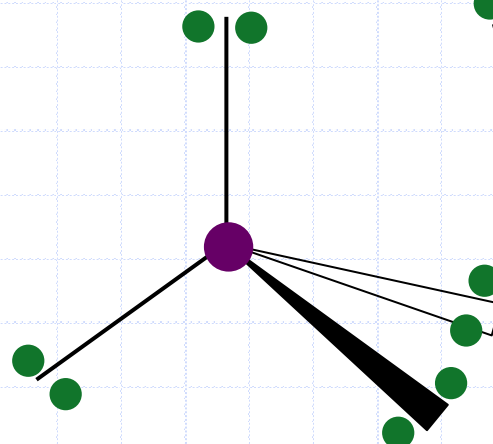
2 - Linear



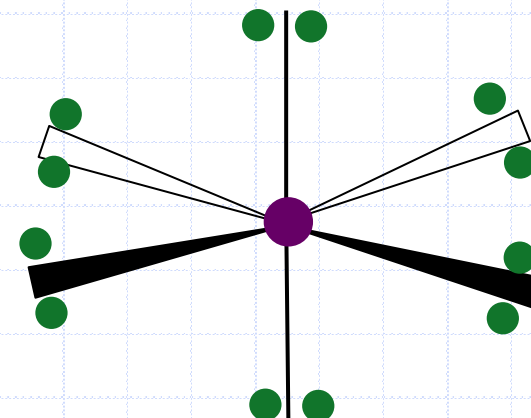
3 - Trigonal Planar



5 - Trigonal Bipyramidal



4 - Tetrahedral

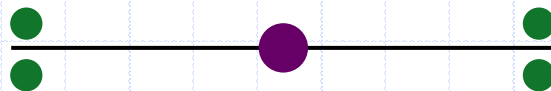


6 - Octahedral



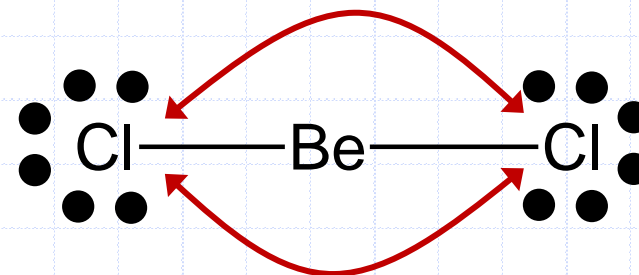
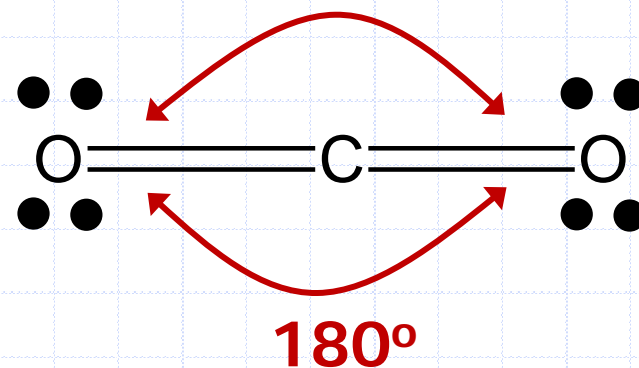
It DOES make a difference if these negative charge centers are lone pairs, bonding pairs, or multiple bonding pairs

2 – Charge Centers

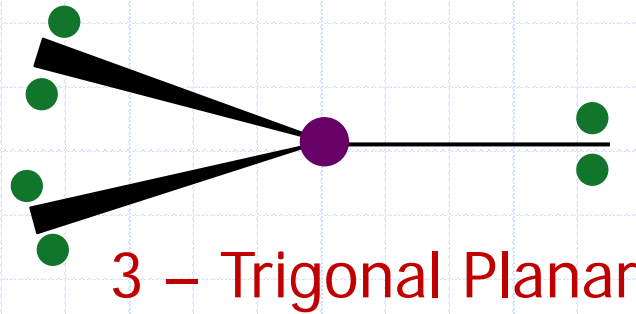


2 - Linear

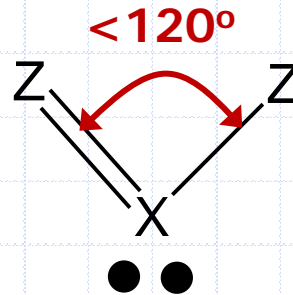
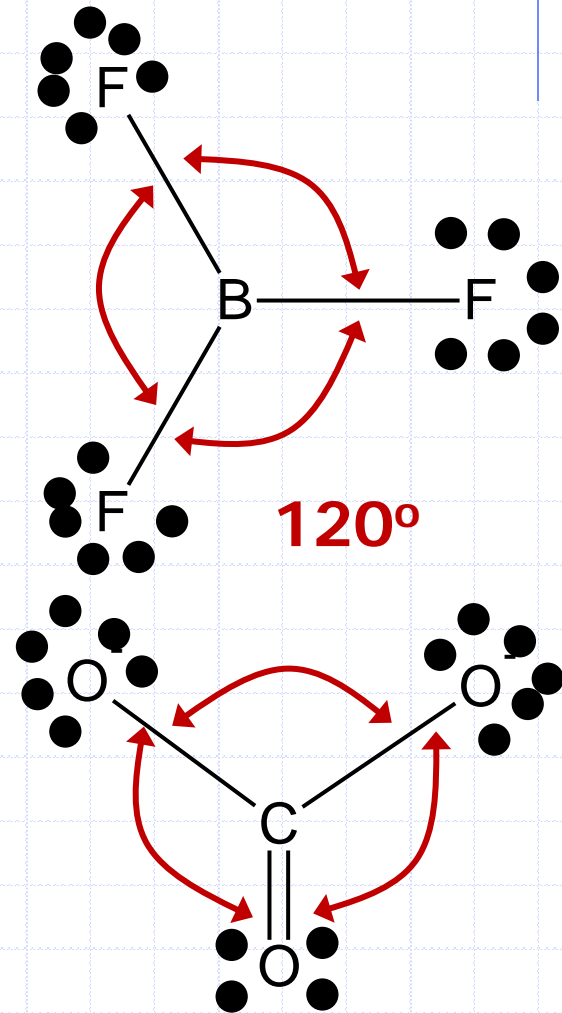
- Whether single, double, or triple bonds, when there are only two charge centers the bond angle must be 180°



3 – Charge Centers

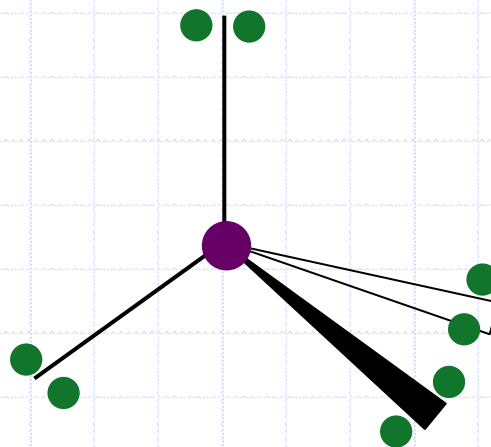


- With three charge centers, the shape will adopt a 120° bond angle
- A double bond would repel more. In the case of CO_3^{2-} the bond resonates, so all are still 120°
- If one center is a lone pair, the other angles are $< 120^\circ$

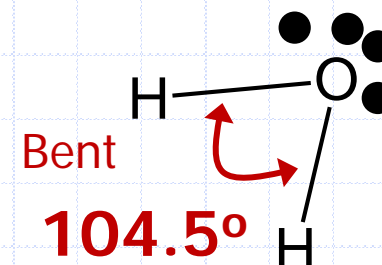
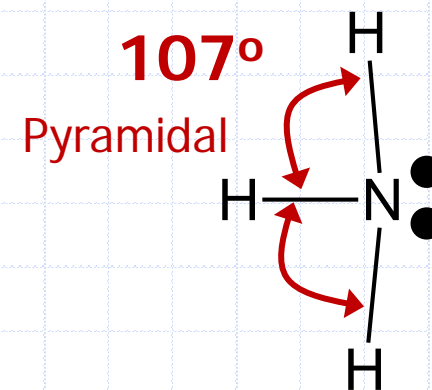
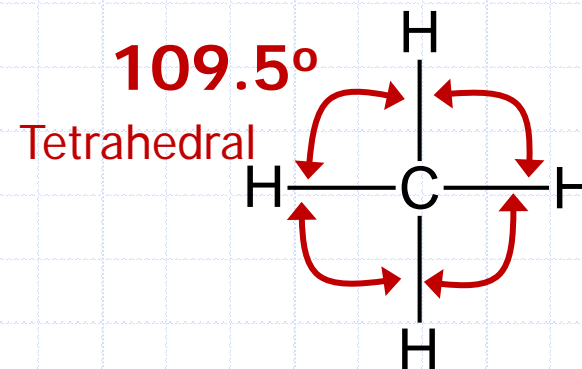


4 – Charge Centers

- L.P.-L.P > B.P.-B.P.
- Four bonding pairs is Tetrahedral
- 3 Bonds + 1 Lone is Pyramidal
- 2 Bonds + 2 Lone is Bent

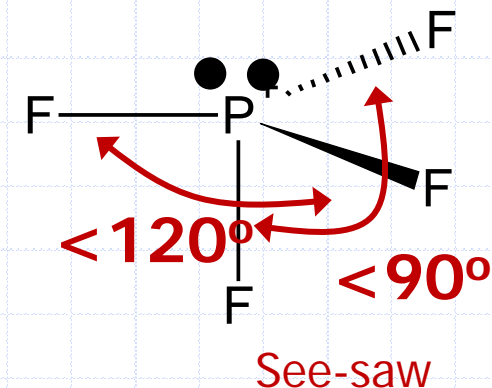
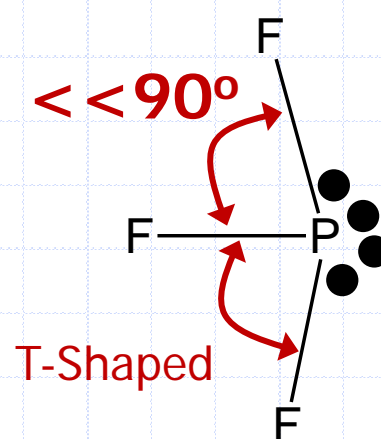
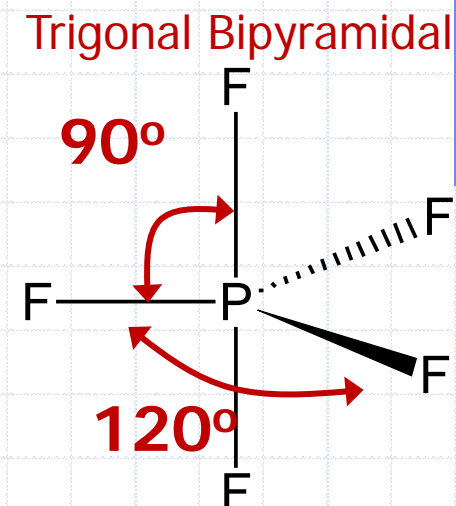
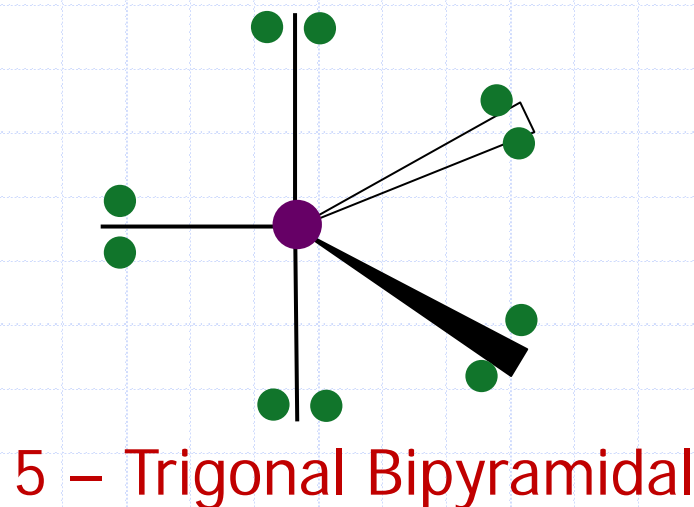


4 - Tetrahedral



5 – Charge Centers

- The more lone pairs, the smaller the bond gets
- HL:
 - See-saw
 - T-shaped

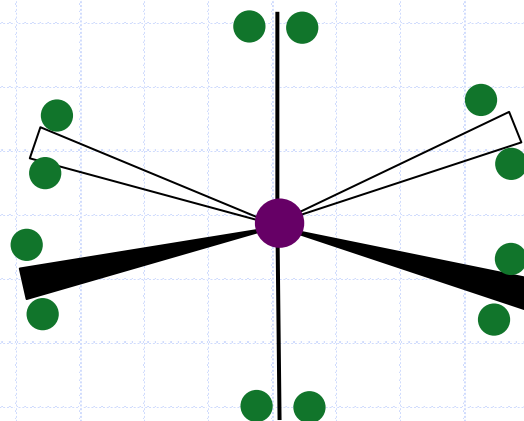


6 – Charge Centers

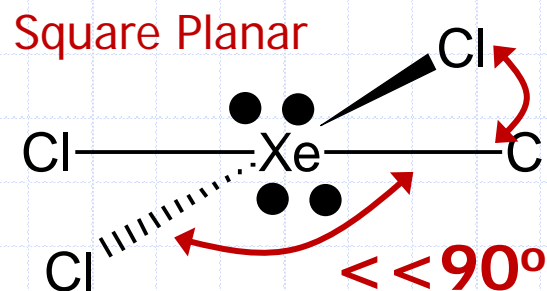
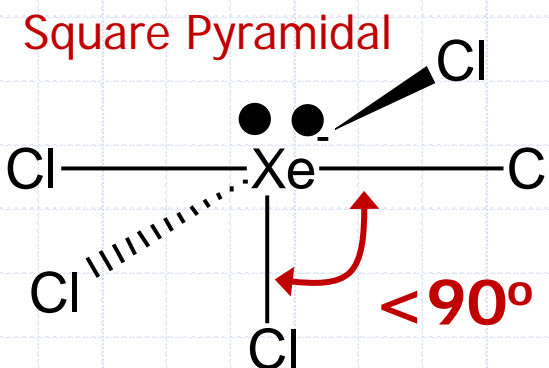
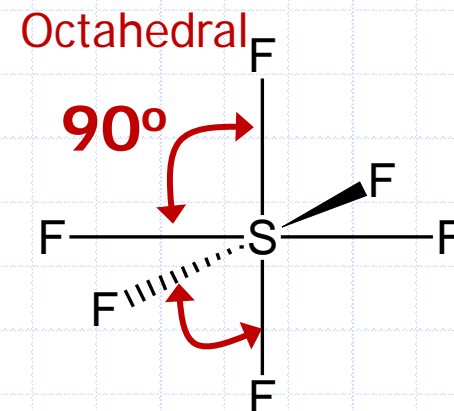
- The more lone pairs, the smaller the bond gets

■ HL:

- Square Pyramidal
- Square Planar



6 - Octahedral

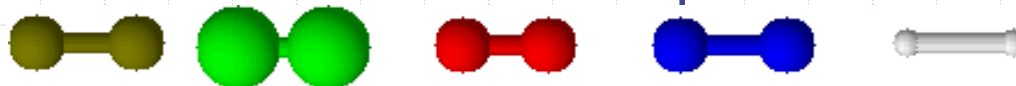


4.2

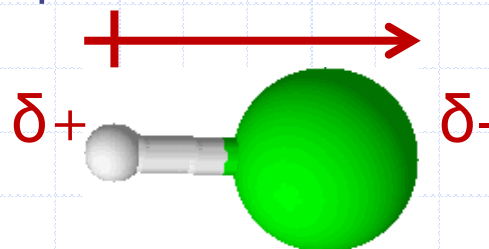
Polarity based on Shape

4.2.8 Predict whether or not a molecule is polar from its molecular shape and bond polarities. (3)

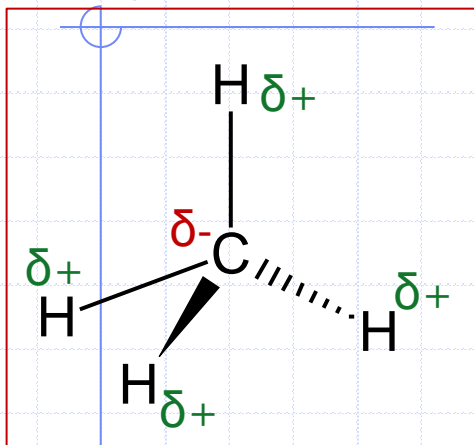
- **BOND** polarity is determined by the difference in electronegativity between two atoms
- The polarity of **MOLECULES** is determined by the shape and symmetry of a molecule
 - Diatomics (Br_2 , I_2 , N_2 , Cl_2 , H_2 , O_2 , F_2) consist of identical elements and are therefore non-polar



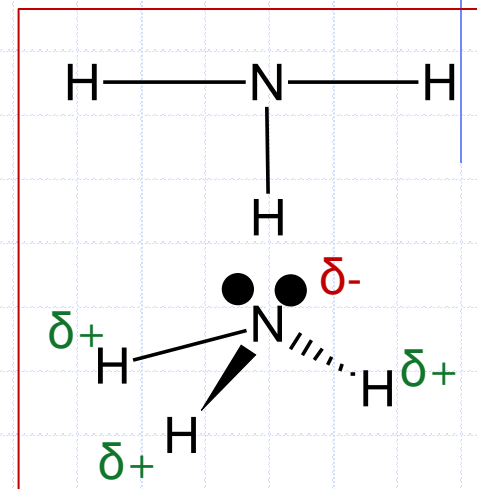
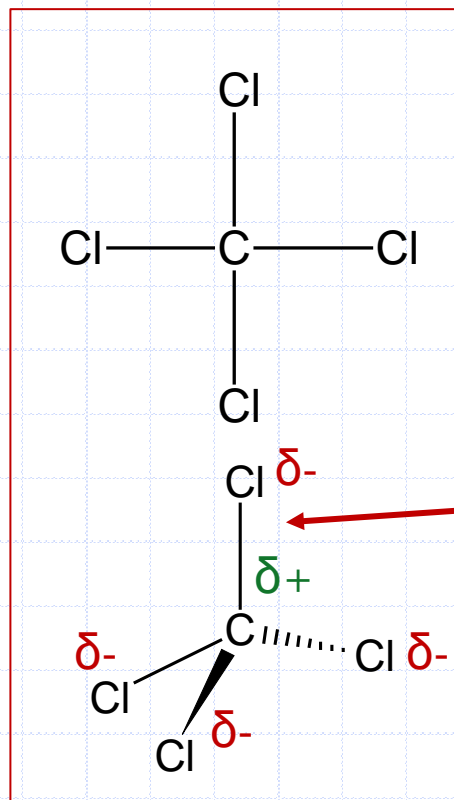
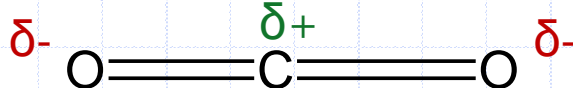
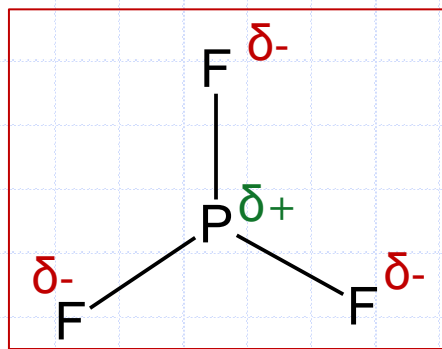
- Compounds such as HCl are polar as there is a difference in electronegativity and size
 - We therefore represent in δ^- and δ^+ to show polarization



Polarity of Molecules

CH₄ (non-polar)

Symmetrical = Non-Polar
Asymmetrical = Polar

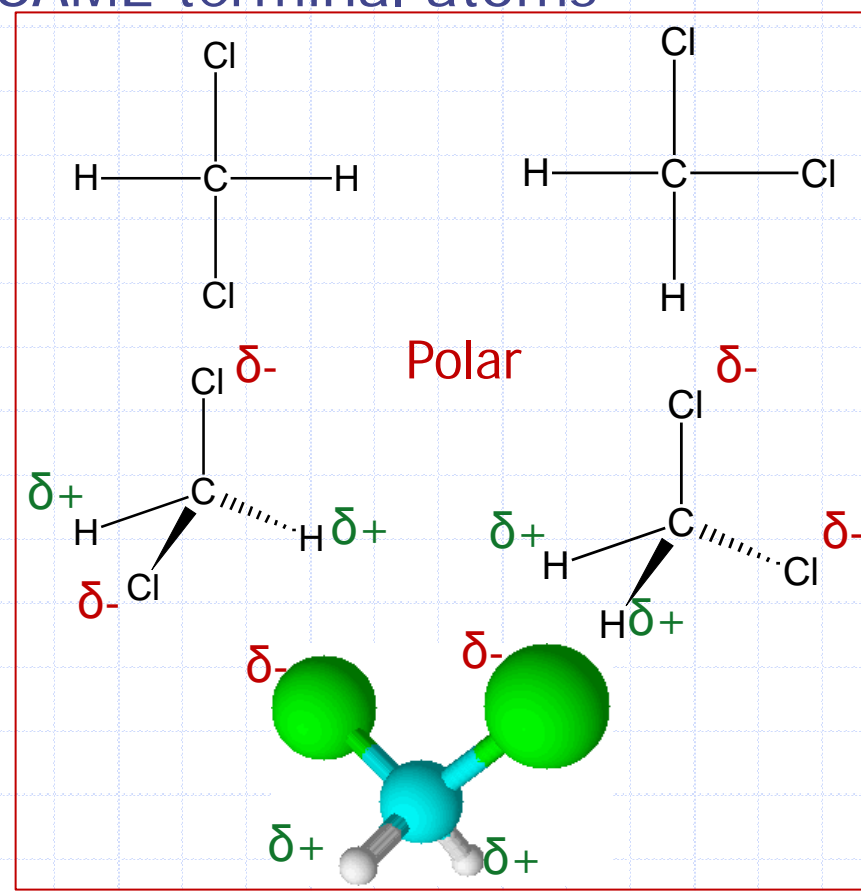
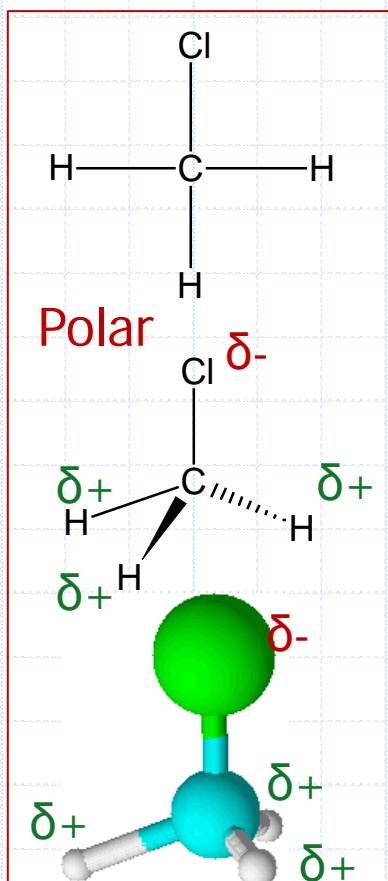
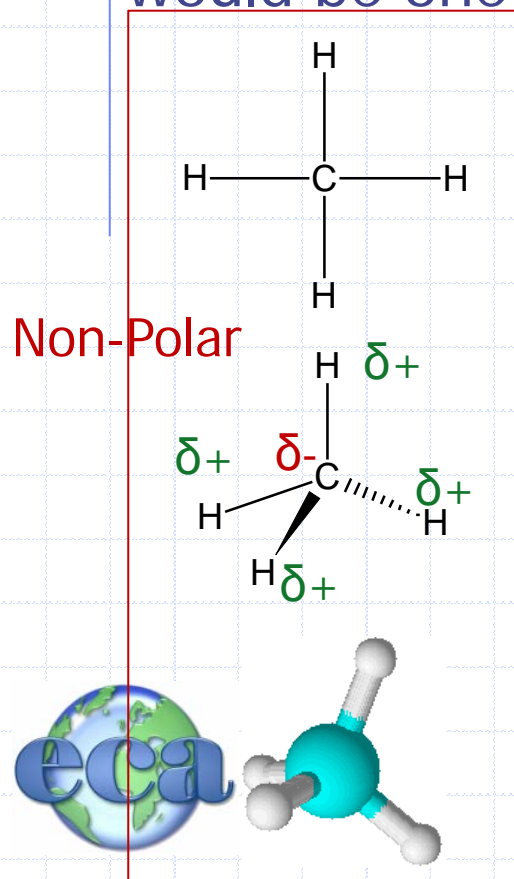
CCl₄ (non-polar)NH₃ (Polar)CO₂ (non-polar)PF₃ (non-polar)

Polar Bonds,
but a non-polar
molecule!!



Polarity of Tetrahedral molecules

- Use care when determining symmetry, you must picture or build the 3-D model!
- With a tetrahedral structure, the only non-polar molecule would be one with four of THE SAME terminal atoms



4.2

Allotropes of Carbon

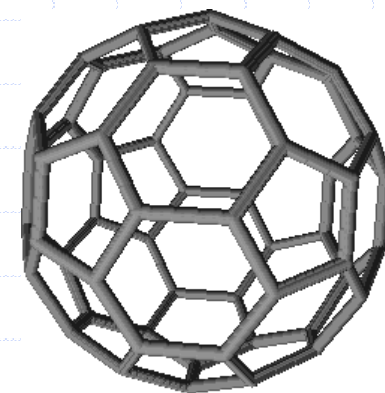
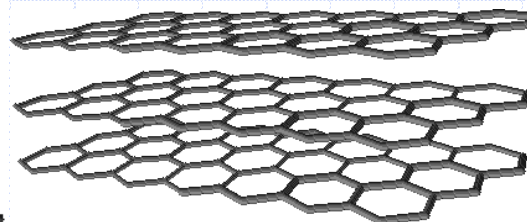
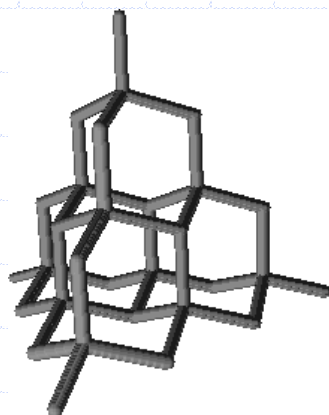
4.2.9 Describe and compare the structure and bonding in the three allotropes of carbon (diamond, graphite and C₆₀ fullerene). (3)

- **Giant Covalent** lattices consist of a 3-D lattice of covalently bound atoms.
 - Same element like Carbon or Silicon
 - Different elements like Silicon Dioxide
- **Allotropes** are crystalline forms of the same element in which the atoms (or molecules) are bonded differently
- Pure Carbon exists in three allotropic forms
 - Diamond
 - Graphite
 - Fullerenes (C-60, C-70, etc)



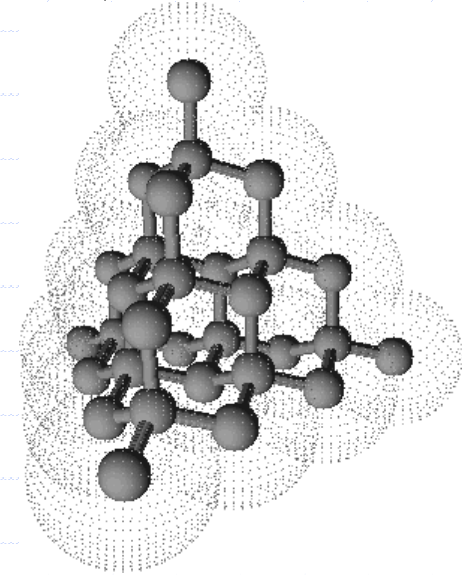
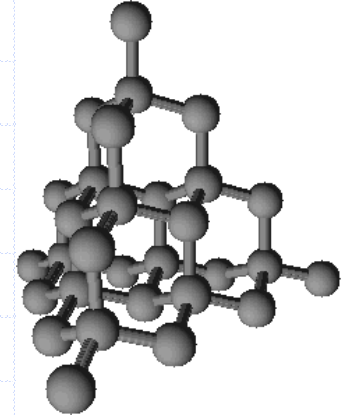
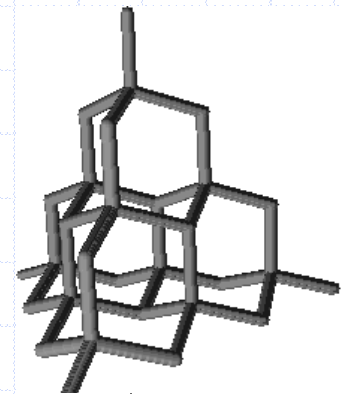
Properties of C Allotropes

Allotrope	Diamond	Graphite	Carbon C-60
Color	Colorless	Black/Opaque	Black
Hardness	Very hard	Very soft and slippery	Soft
Electrical Conductivity	Very poor = insulator	Good – along the plane of layers	Very poor = insulator
Density (g cm ⁻³)	3.51	2.23	1.72
Melting Point (K)	3823	Sublimes (3925-3970)	Sublimes 800
Boiling Point (K)	5100	" "	" "



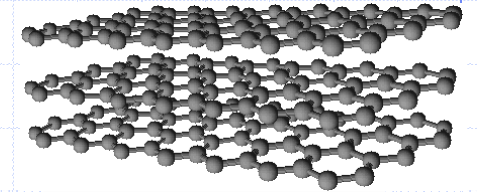
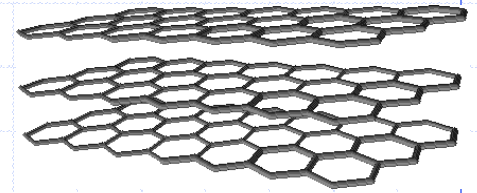
Diamond

- In Diamond, each carbon atom is tetrahedrally bonded to four other carbon atoms
 - All single bonds
 - Very ridged 3-D network is formed
 - Bond angles are 109.5°
 - Each C has a coordination number of 4
- Non-conductive but can go through a process called “doping” in which small amounts of other atoms are added.



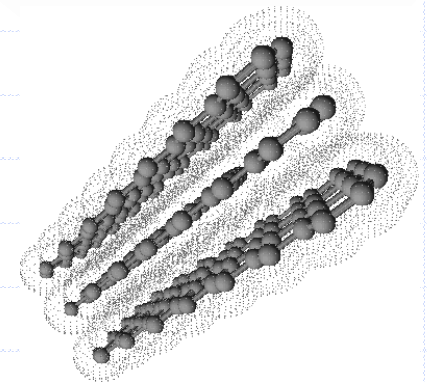
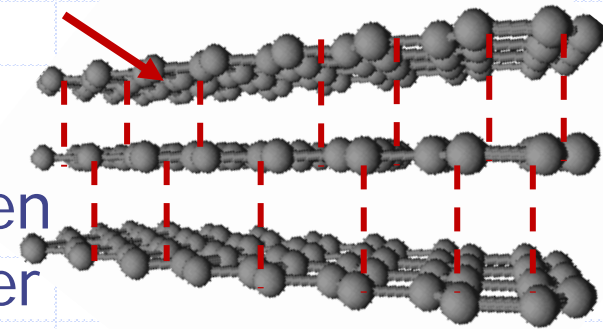
Graphite

- Each carbon is covalently bonded to only three other C-atoms
- 2-D ring of hexagonal rings of C-atoms is formed



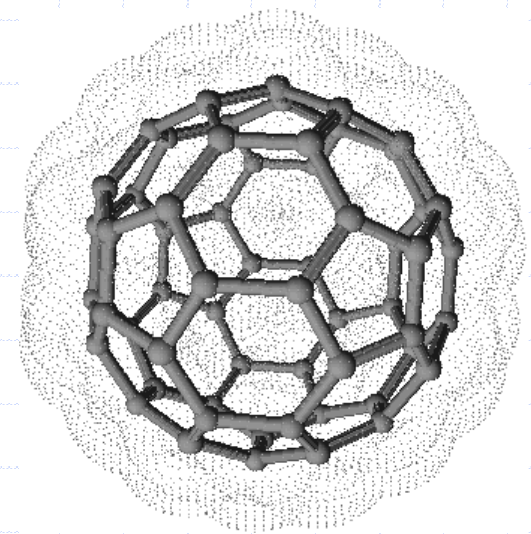
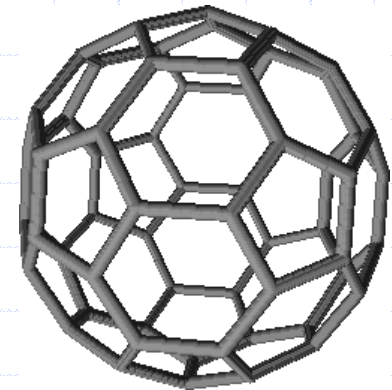
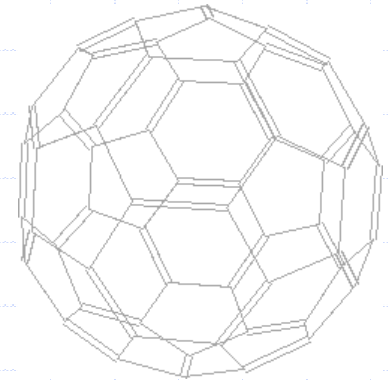
- A graphite crystal has many of these stacked on top of each other
- There is NO covalent bonding between the stacks as they are held by Van der Waals forces alone
- Spare electron?
 - Each carbon donates the spare electron (becoming delocalized) which accounts for the electrical conductivity

Van der Waals Forces



Fullerenes

- Also known as a Bucky-ball
- Arranged into a shape of a truncated icosahedron (soccer/football)
- The structure has
 - 60 Carbons (corners)
 - 32 Faces
 - 12 pentagons (none are adjacent)
 - 20 hexagons
 - Alternating single and double bonds



4.2

Silicon Structures and Network Covalent

4.2.10 Describe the structure of and bonding in silicon and silicon dioxide. (2)

- The most common form of silicon dioxide (silica) is quartz which is similar to diamond
 - SiO_4 groups are bonded by Si-O-Si bonds
 - Has physical properties very similar to diamond
 - Very hard and transparent with high melting and boiling points
- Common, impure form is sand which is colored yellow by iron (II) oxide

Silicon itself can also form a giant covalent structure similar to diamond. It's less hard as it has larger atoms with longer and weaker bonds. It is an insulator like diamond (unless doped).

